Integrated density of states of Schrödinger operators with periodic or almost-periodic potentials

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Joint work with Roman Shterenberg (Birmingham Alabama)

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acting in $\mathbb{R}^d$. The potential $b = b(\mathbf{x})$ is assumed to be real, smooth, and either periodic, or almost-periodic. The density of states of H can be defined by the formula

$$N(\lambda) = N(\lambda; H) := \lim_{L\to\infty} \frac{N(\lambda; H_D^{(L)})}{(2L)^d}.$$

Here, $H_D^{(L)}$ is the restriction of H to the cube $[-L, L]^d$ with the Dirichlet boundary conditions, and $N(\lambda; A) = \#\{\lambda_j(A) \leq \lambda\}$ is the counting function of the discrete spectrum of A.

To begin with, let us assume that the potential b is periodic with lattice of periods Γ. Let $\Gamma^\dagger$ be the dual lattice to Γ. Then we can perform Floquet-Bloch decomposition and express the operator H as a direct integral

$$H = \int_{\oplus} H(\mathbf{k}) d\mathbf{k},$$

quasi-momentum $\mathbf{k}$ running over $\mathbb{R}^d/\Gamma^\dagger$. Here, $H(\mathbf{k}) = (i\nabla + \mathbf{k})^2 + b$ acting in $L^2(\mathbb{R}^d/\Gamma)$. Then we can express the density of states as

$$N(\lambda) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d/\Gamma^\dagger} N(\lambda, H(\mathbf{k})) d\mathbf{k}.$$

If we put $H_0 = -\Delta$, for positive λ we have

$$N(\lambda; H_0) = C_d \lambda^{d/2},$$

where

$$C_d = \frac{w_d}{(2\pi)^d}$$

and

$$w_d = \frac{\pi^{d/2}}{\Gamma(1 + d/2)}$$

is a volume of the unit ball in $\mathbb{R}^d$.

There is a long-standing conjecture that the density of states of H enjoys the following asymptotic behaviour as $\lambda \to \infty$:

$$N(\lambda) \sim \lambda^{d/2}\Big(C_d + \sum_{j=1}^{\infty} e_j \lambda^{-j}\Big), \tag{1}$$

meaning that for each $K \in \mathbb{N}$ one has

$$N(\lambda) = \lambda^{d/2}\Big(C_d + \sum_{j=1}^{K} e_j \lambda^{-j}\Big) + R_K(\lambda) \tag{2}$$

with $R_K(\lambda) = o(\lambda^{\frac{d}{2}-K})$.

The coefficients e_j are real numbers which depend on the potential b. They can be calculated using the heat kernel invariants, computed by Polterovich, Hitrik-Polterovich, and Korotyaev-Pushnitski; they are equal to a certain integrals of the potential b and its derivatives. For example,

$$e_1 = -\frac{dw_d}{2(2\pi)^d|\mathbb{R}^d/\Gamma|}\int_{\mathbb{R}^d/\Gamma} b(\mathbf{x})d\mathbf{x}$$

and

$$e_2 = \frac{d(d-2)w_d}{8(2\pi)^d|\mathbb{R}^d/\Gamma|}\int_{\mathbb{R}^d/\Gamma} (b(\mathbf{x})^2)d\mathbf{x}.$$

Formula (1) was proved in the case $d = 1$ by Shenk-Shubin (1987) and $d = 2$ by L.P.-Roman Shterenberg (2009)

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If $d \geq 3$, only partial results are known, works by Skriganov, Karpeshina, Helffer, Mohamed, Veliev, Sobolev, Knörrer, Trubowitz, L.P.

In particular, Yu.Karpeshina showed that when $d = 3$, formula (2) is valid with $K = 1$ and $R(\lambda) = O(\lambda^{-\delta})$ with some small positive δ and $R(\lambda) = O(\lambda^{\frac{d-3}{2}} \ln \lambda)$ when $d > 3$.

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If b is almost-periodic and $d = 1$, formula (1) was proved by Savin (1988). For $d \geq 2$, (2) is known only with $K = 0$ and $R(\lambda) = O(\lambda^{\frac{d-2}{2}})$ (Shubin, 1987).

Theorem.

Formula (1) *is valid for smooth periodic b and arbitrary d.*

Let b be either quasi-periodic:

$$b(\mathbf{x}) = \sum_{\theta \in \Theta} a_\theta e^{i\theta \mathbf{x}}$$

(Θ being a finite set), or almost-periodic (a uniform limit of quasi-periodic functions).

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$$\mathbf{M}(b) := \lim_{L \to \infty} \frac{\int_{[-L,L]^d} b(\mathbf{x}) d\mathbf{x}}{(2L)^d}$$

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exists and is called the mean of b. For each $\theta \in \mathbb{R}^d$ we define the Fourier coefficient

$$a_\theta = a_\theta(b) := \mathbf{M}_\mathbf{x}(b(\mathbf{x}) e^{-i\theta \mathbf{x}})$$

and the spectrum $\Theta(b) := \{\theta \in \mathbb{R}^d,\ a_\theta \neq 0\}$.

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Condition A. Suppose that $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_d \in Z(\boldsymbol{\Theta})$. Then $Z(\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_d)$ is discrete.

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This condition can be reformulated like this: suppose, $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_d \in Z(\boldsymbol{\Theta})$.Then either $\{\boldsymbol{\theta}_j\}$ are linearly independent, or $\sum_{j=1}^d n_j \boldsymbol{\theta}_j = 0$, where $n_j \in \mathbb{Z}$ and not all n_j are zeros.

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Theorem.

Formula (1) *is valid for quasi-periodic b satisfying Condition A.*

Suppose, b is almost-periodic. Let $k \in \mathbb{N}$ be arbitrary. We require that for each sufficiently small ϵ there exists a quasi-periodic potential

$$\tilde{b}(\mathbf{x}) = \sum_{\theta \in \tilde{\Theta}} \tilde{a}_\theta e^{i\theta\mathbf{x}}$$

so that

$$||b - \tilde{b}||_\infty < \epsilon.$$

Let $\tilde{\Theta}_k := \tilde{\Theta} + \tilde{\Theta} + \cdots + \tilde{\Theta}$ (algebraic sum taken k times). We require $\sup_{\theta \in \tilde{\Theta}_k} |\theta| \ll \epsilon^{-1/k}$, $\inf_{\theta \in \tilde{\Theta}_k, \theta \neq 0} |\boldsymbol{\theta}| \gg \epsilon^{1/k}$. We also require that the angles between all subspaces spanned by elements of $\tilde{\Theta}_k$ are bounded below by $C\epsilon^{1/k}$.
Let $\theta_1, \ldots, \theta_m \in \tilde{\Theta}_k$, $m < d$. Denote by $\mathfrak{V}$ the linear span of these vectors and put $\Gamma_{\mathfrak{V}} := Z(\tilde{\Theta}_k \cap \mathfrak{V})$. Condition A implies that $\Gamma_{\mathfrak{V}}$ is discrete. Our final requirement is: $|\mathfrak{V}/\Gamma_{\mathfrak{V}}| \gg \epsilon^{1/k}$.

Theorem.

Formula (1) *is valid for almost-periodic b satisfying Condition A and all the above conditions.*

The coefficients are computed by similar formulas, e.g.

$$e_1 = -\frac{d w_d}{2(2\pi)^d}\mathbf{M}(b)$$

and

$$e_2 = \frac{d(d-2)w_d}{8(2\pi)^d}\mathbf{M}(b^2)$$

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Actually, we prove the following formula:

$$N(\rho^2) = C_d\rho^d + \sum_{p=0}^{d-1}\sum_{j=-d+1}^{K} e_{j,p}\rho^{-j}(\ln\rho)^p + o(\rho^{-K}),$$

but most of the coefficients turn out to be zero due to Hitrik-Polterovich.

What is the analogue of the formula

$$N(\lambda) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d/\Gamma^\dagger} N(\lambda, H(\mathbf{k}))d\mathbf{k}$$

for almost-periodic b? There are two definitions, and we need them both!

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Definition 1:
In all points of continuity of N, we have:

$$N(\lambda) = \mathbf{M}_{\mathbf{x}}(e(\lambda; \mathbf{x}, \mathbf{x})),$$

where $e(\lambda; \mathbf{x}, \mathbf{y})$ is the integral kernel of the spectral projection of H.

Definition 2 (cheating)

$$N(\lambda) = \mathbf{T}(E_\lambda(\tilde{H})) = \mathbf{D}(E_\lambda(\tilde{H})L^2(\mathbb{R}^d)).$$

Here, **T** is the regularized (von Neumann) trace, and **D** is the relative dimension.

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In particular, $N(\lambda; H) = N(\lambda; U^{-1}HU)$, where U is a unitary operator with almost-periodic coefficients.

Another useful trick: often, we work with operators acting not in $L_2(\mathbb{R}^d)$, but in $B_2(R^d)$ (Besicovitch space). This is a collection of all formal sums

$$\sum_j a_j e^{i\theta_j \mathbf{x}}$$

with

$$\sum_j |a_j|^2 < +\infty.$$

This is a non-separable Hilbert space. Results of Shubin show that the norms and spectra of almost-periodic operators acting in $L_2(\mathbb{R}^d)$ and $B_2(R^d)$ are often the same.

Assume now for simplicity that b is periodic. There are two methods of obtaining information of the eigenvalues of $H(\mathbf{k})$. The first method is called the method of spectral projections. Let $\{P_j\}$ be spectral projections of H_0 (i.e. they are projections commuting with H_0) so that $\sum P_j = I$. We look at the operator

$$\tilde{H} = \sum_j P_j H P_j.$$

If we choose the projections P_j very carefully, then the spectra of H and $\tilde{H}$ are close to each other.

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If we choose the projections P_j very carefully, then the spectra of H and $\tilde{H}$ are close to each other.

The second method is called the method of gauge transform. We look at the operator

$$H_1 = e^{-i\Psi} H e^{i\Psi}.$$

After carefully choosing bounded pseudo-differential almost-periodic operator Ψ, we can achieve that H_1 is norm-close to the operator H_2 which is 'almost' diagonal and so has many invariant subspaces.

Both methods produce two types of invariant subspaces (of $\tilde{H}$ or H_2): stable (corresponding to perturbations of simple eigenvalues, lying not too close to other eigenvalues) and unstable (corresponding to perturbations of a cluster of eigenvalues lying close together). It is straightforward to compute the contribution to the density of states from the stable subspaces. Unstable eigenvalues cause the main problem.

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Both methods reduce operator acting in unstable subspaces to the form

$$r^2 I + S(r),$$

where $r \sim \lambda^{1/2}$ and $S(r)$ is a self-adjoint finite-dimensional operator with (almost explicitly written) analytic symbol.

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We can use the expansion

$$\lambda(A + \varepsilon B) \sim \sum \lambda_j \varepsilon^j,$$

but we cannot integrate it against $d\mathbf{k}$, since the coefficients λ_j can be unbounded functions of $\mathbf{k}$.

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In our previous paper, we have shown that if $d = 2$, we have

$$\lambda(A + \varepsilon B) \sim \sum \varepsilon^j \lambda_j \pm \sqrt{\sum \varepsilon^j \tilde{\lambda}_j},$$

where the coefficients λ_j and $\tilde{\lambda}_j$ are bounded functions of the quasi-momentum and so can be integrated against $d\mathbf{k}$.

Now we use the method of gauge transform. Then $S(r)$ does not have a nice form, but we need to compute the contribution from all eigenvalues of $r^2 I + S(r)$, whereas before we had to separate the eigenvalues contributing to the density of states from the rest of eigenvalues. Since $||S'(r)|| < r/2$, each eigenvalue $\lambda_j(r^2 I + S(r))$ is an increasing function of r. Thus, the equation

$$r^2 + \lambda_j(S(r)) = \lambda =: \rho^2$$

has a unique solution, denoted by τ_j. The contribution to the density of states equals

$$\sum_j \tau_j^m,$$

where $m \in \mathbb{N}$.

Let γ be a contour in the complex plane containing all points τ_j. The points τ_j are singularities of $\det[S(z) + z^2 I - \rho^2 I]$. Using

$$\mathrm{tr}[F'(z)F^{-1}(z)] = (\det[F(z)])'(\det[F(z)])^{-1}$$

and the residue theorem, we obtain:

$$
\begin{aligned}
&\sum_j \tau_j^m \\
&= \frac{1}{2\pi i}\oint_\gamma z^{m+1}(\det[S(z)+z^2I-\rho^2 I])'(\det[S(z)+z^2I-\rho^2 I])^{-1}dz \\
&= \frac{1}{2\pi i}\oint_\gamma \mathrm{tr}[z^{m+1}(2zI+S'(z))(S(z)+z^2I-\rho^2 I)^{-1}]dz \\
&= \frac{1}{2\pi i}\oint_\gamma \mathrm{tr}[(2z^{m+2}I+z^{m+1}S'(z))(z^2-\rho^2)^{-1}\sum_{l=0}^{\infty}(-1)^l S^l(z)(z^2-\rho^2)^{-l}]dz \\
&= \frac{1}{2\pi i}\sum_{l=0}^{\infty}(-1)^l\oint_\gamma \mathrm{tr}[(2z^{m+2}I+z^{m+1}S'(z))S^l(z)(z-\rho)^{-(l+1)}(z+\rho)^{-(l+1)}]dz \\
&= \sum_{l=0}^{\infty}\frac{(-1)^l}{l!}\,\mathrm{tr}\,\frac{d^l}{dr^l}[(2r^{m+2}I+r^{m+1}S'(r))S^l(r)(r+\rho)^{-(l+1)}]\Big|_{r=\rho}\ .
\end{aligned}
$$